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Prospects for a Special-Purpose Lattice Gas Computer

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A two-day workshop was held in June of 1988, to discuss the feasibility of designing and building a large special-purpose computer dedicated to lattice-gas cellular automata. The primary emphasis was on applications of cellular automata for modeling Navier-Stokes hydrodynamics. The meeting had two goals: 1) To identify those theoretical issues which would have to be addressed before the hardware implementation of a lattice-gas machine would be possible; and 2) To begin to evaluate alternative architectures for a dedicated lattice-gas computer. This brief paper contains a summary of the main issues and conclusions discussed at the workshop.

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Abstract

A two-day workshop was held in June of 1988, to discuss the feasibility of designing and building a large special-purpose computer dedicated to lattice-gas cellular automata. The primary emphasis was on applications of cellular automata for modeling Navier-Stokes hydrodynamics. The meeting had two goals: 1) To identify those theoretical issues which would have to be addressed before the hardware implementation of a lattice-gas machine would be possible; and 2) To begin to evaluate alternative architectures for a dedicated lattice-gas computer. This brief paper contains a summary of the main issues and conclusions discussed at the workshop.

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1 INTRODUCTION

This note summarizes a two-day workshop held in La Jolla, California in June of 1988. The workshop was cosponsored by the Center for Nonlinear Studies at the Los Alamos National Laboratory, and by the JASON group, The MITRE Corporation as part of the 1988 JASON Summer Study. The purpose of the workshop was to identify, define, and begin to resolve substantive issues which must be addressed before a special purpose cellular automata computer can be implemented in hardware.

The workshop attendees were:

- George Adams, Purdue University
- Gary Doolen, Los Alamos National Laboratory
- Paul Frederickson, NASA Ames, RIAC project
- Castor Fu, Stanford University
- Brosl Hasslacher, Los Alamos National Laboratory
- Fung F. Lee, Stanford University
- Norman Margolus, MIT Laboratory for Computer Science
- Tsutomu Shimomura, Los Alamos National Laboratory
- Tom Toffoli, MIT Laboratory for Computer Science

and the following members of the JASON group:

- Kenneth Case, University of California at San Diego
- Alvin Despain, University of California at Berkeley
- Freeman Dyson, Institute for Advanced Study
- Michael Freedman, University of California at San Diego
- Claire Max, Lawrence Livermore National Laboratory

- Oscar Rothaus, Cornell University.

Henry Abarbanel, a JASON from the University of California at San Diego, was not able to attend the two day workshop, but did participate in planning the workshop and in discussion of issues.

The primary emphasis of the workshop was on the use of cellular automata for simulations of three-dimensional incompressible Navier-Stokes hydrodynamics. Within this context, there are two types of applications for which a special purpose computer might offer important potential advantages over conventional numerical hydrodynamics techniques implemented on general purpose supercomputers:

1. Studies of flows with complex boundary conditions. For example, one might look at a boundary-layer and study various techniques that have been suggested for drag-reduction and boundary-layer modification.

2. Studies of three-dimensional incompressible flows at high Reynolds numbers. These could include studies of the onset of fluid turbulence, free-boundary problems (such as ship wakes and drag), or the combination of hydrodynamics and simple chemical reaction systems.

The issues discussed at the workshop fall into three general categories: theory, computer simulation, and hardware.

2 THEORETICAL ISSUES

The most prevalent use of cellular automata for modeling hydrodynamics has been the so-called lattice gas. In this approach, one follows the motions of many individual particles which interact via given collision laws at fixed lattice sites or nodes. The individual particles are allowed to have at most a few discrete speeds relative to the grid of lattice nodes. The hydrodynamic limit is regained by averaging over a large number of these discrete particles, to obtain the first few moments of their distribution function; namely, the fluid velocity, density, etc. In two spatial dimensions, the properties of possible sets of collision rules for the particles and lattice geometries for the nodes are now reasonably well understood. There are two practical ways to represent a given rule set: via a look-up table which enumerates all the possible incoming and outgoing configurations, or via an algorithm or computation which generates the rules anew at each timestep and each collision site.

However in three spatial dimensions the possible rules sets are far more complicated, and there are many unsolved questions regarding appropriate collision rules and their efficient execution. For maximum efficiency, a special-purpose lattice-gas computer should probably contain a hard-wired implementation of a particular rule set. However the general consensus at the workshop was that there is not yet a sufficient understanding of rule sets that have been proposed for three spatial dimensions to settle upon an optimum one for hardware implementation.

Important issues that remain to be solved concerning collision rules for three-dimensional hydrodynamics are the following:

1. What is the "best" rule set to use for modeling three-dimensional hydrodynamics?

   (a) How does the choice of this "best" rule set change with the type of application one wants to solve? For example, are some rule sets better for studies of boundary-layer effects of free-boundary problems, while others are optimum for studying the onset of turbulence at high Reynolds number?

(b) How can rules be "tuned" to get optimum results for given problem parameters? For example, how can one optimize for high Reynolds number, or for specific types of boundary conditions?

2. Rules for lattice gases representing three-dimensional hydrodynamics tend to be very complicated. One way to implement them computationally is using a look-up table, but these become very large. If there are n bits at each lattice site, then there are 2^n table entries. For example, the 24 bit model requires 16 million entries. How can this large number of rules be reduced by "factoring" or "grouping" them, to reduce the size of the rule representation in the look-up table? What is the fundamental dimension of the rule set?

3. In several proposed rule sets, one has to choose whether the same collision will always have the same outcome, or whether one will implement a randomization process within the rule set to "mix up" the collision outcomes. The addition of an explicit randomization procedure is expensive computationally. Under what circumstances can one rely on the inherently high frequency of particle collisions to achieve randomization, so that it does not have to be explicitly included in the rule engine?

4. A related question concerns the desirability of adding a "collision bit" to the algorithm. This is an additional bit determining whether a particle will or will not undergo a collision at the next lattice node that it reaches, if all the other conditions for a collision at that node are satisfied. If all particles undergo collisions whenever they can (no collision bit), one obtains a more "collisional" rule set, leading to the potential for attaining higher Reynolds numbers. Are there circumstances in which a less collisional rule set would be desirable?

5. What advantages are there to using non-periodic tiling or quasilattices for modeling three-dimensional hydrodynamics, as compared with the so-called four-dimensional schemes or other periodic tiling schemes?

6. Is there a lattice-gas analog for adaptive-mesh hydrodynamic techniques, so that greater spatial resolution can be achieved in regions where it is needed? Can sub-grid scaling rules be derived to extend the spatial resolution of the lattice gas method?

7. What physical laws or partial differential equations do the various rule sets represent? Can the differences between the Navier-Stokes equations and the lattice gas implementations be systematically understood?

   (a) Under what conditions (limits on the Mach number, particle density, Reynolds number) does the lattice gas model with a given rule set reduce to three-dimensional Navier-Stokes hydrodynamics?

   (b) Given a set of physical constraints, can an algorithm be developed that will systematically generate a corresponding lattice gas rule set?

   (c) Each given rule set implies a particular functional form for the viscosity as a function of density. Given that the density is nearly constant in space for incompressible flows with Mach numbers small compared to unity, does it matter whether or not the density-dependence of the viscosity law is physical?

   (d) It has been suggested that the nonphysical function $g(\rho)$ appearing in front of the $u \cdot \nabla u$ term in the momentum equation can be eliminated by using rules which include two or more discrete (nonzero) velocities. Is this generally valid? Under what conditions would it be desirable to use more than one particle velocity? What is the gain in accessible Reynolds number when additional speeds are allowed? Are there advantages to these schemes that would allow lattice gases to satisfy statistics other than Fermi statistics? (The latter prevail for most currently used rules.)

In addition to the above questions concerning rules for lattice-gas representations of hydrodynamics, there are a set of issues involving extensions of the cellular automata methodology to other physical models:

   (a) Can hydrodynamics be modeled by using cellular automata particles to represent vorticity, in analogy with finite-difference vorticity-tracking algorithms? What range of Reynolds numbers could such a technique model?

   (b) How practical would it be to add some simple extensions to three-dimensional lattice-gas hydrodynamics? Some extensions that would be useful include gravity or other body-forces, two or more different fluid types, or simple chemistry. It was generally agreed

at the workshop that extensions which involve action-at-a-distance, such as Maxwell's equations, would require a very different algorithmic approach.

3 ISSUES CONCERNING NUMERICAL SIMULATIONS

The workshop participants felt that there was a need to develop "benchmark" simulation problems. These would consist of a few canonical two and three-dimensional hydrodynamics problems, for which the numerical results of various lattice-gas models could be compared with each other, with conventional hydrodynamics simulations, and with experimental results. This is particularly important because of the fact that different lattice-gas rule sets may represent different approximations to the Navier-Stokes equations (i.e., they may approach the Navier-Stokes equations in different asymptotic limits).

A parallel effort should be made to compare lattice-gas simulation results with standard analytic solutions to the Navier-Stokes equations, in cases where these are known. Possible examples are channel flow, pipe flow, Pouseille flow, Couette flow, and so forth. This has been done to a limited extent for two-dimensional lattice-gas models, but three-dimensional applications have not yet been well studied.

A different type of test of lattice-gas algorithms was thought to be important as well. One should perform the standard numerical test of increasing the grid resolution, while holding fixed all of the "physical" parameters describing the problem. The goal would be to check that the higher-resolution result is identical to that obtained with lower numerical resolution.

A final numerical simulation issue thought to be important by the workshop participants concerns how to generate adequate graphical visualizations of the results of a three-dimensional lattice-gas simulation. It was pointed out that the amount of data storage needed for a three-dimensional simulation at high Reynolds number will be very high. Therefore, thought must be given to how to integrate input-output and graphical display within the process of the numerical computation itself. For the types of physical problems which one wants to address using lattice gases, it may not be adequate to obtain graphical displays of the results based entirely upon post-processing.

4 ISSUES CONCERNING THE HARDWARE PERFORMANCE OF A SPECIAL-PURPOSE LATTICE-GAS COMPUTER

In order to focus on the issue of hardware design for a lattice-gas machine, a set of performance measures was chosen. The idea was to outline hypothetical specifications for hardware components, so that when different candidate architectures were compared with each other, they would all be making the same assumptions about the capabilities of commonly used hardware components. The following table gives a rough overview of the capabilities of VLSI technology today and in 5 years.

Table 1: VLSI Technology (CMOS)

Today	**In Five Years**
1 cm^2 active area	1 cm^2
200 pins	400 pins
1 Mbit DRAM	4 Mbit
50K "random" transistors	200K
10 nsec internal clock (on-chip communications)	1 nsec
80 nsec external drive (off-chip communications)	8 nsec

Using these characteristics, which are of course only approximate, one can outline the characteristics and performance of various architectures for a lattice gas supercomputer.

There appears to be a practical limit on the total number of chips it is plausible to include in a supercomputer. Today's Crays have about a third of a million chips. Workshop participants hypothesized that in the future one might build supercomputers with up to a million chips. Since the total number of lattice points required for a lattice-gas computation of high Reynolds number three-dimensional hydrodynamics is much larger than a

million, one is led to a design in which many cellular automata lattice points are placed on each chip.

The next hardware issue is how to implement the set of collision rules. Since only a few rule sets for three spatial dimensions have been studied to date, the workshop participants felt that it was premature to choose a specific rule set for implementation in hardware. It was suggested that even after more three-dimensional rules have been studied, it would be desirable to leave flexibility in the choice of rules for the lattice-gas supercomputer. There are two reasons for this choice. First, a new and better set of collision rules for hydrodynamics might be invented at any time; and second, one may at some later point want to use the lattice-gas computer to study other physical models such as the mixing of two different gases, or hydrodynamics with simple chemistry.

Flexibility in the choice of rule set would have the most straightforward implementation if collision rules were executed via look-up tables. In that case one could feed an alternative look-up table into the computer when one wanted to change rules. The difficulty with this approach is that the rules suggested to date for hydrodynamics in three spatial dimensions would require very large look-up tables, with the disadvantages that the tables would use up large amounts of memory and would be slow to compute collisions.

Thus there is a lot to be gained by understanding the symmetries underlying each proposed rule set, so that the look-up table can be collapsed into a considerably smaller amount of memory space.

The second method of implementing a rule set is to design a computation engine in hardware that would recalculate the rules "on the fly" for each collision. The advantage of this technique relative to a look-up table approach is that it is preferable from the point of view of speed and feasibility. The hardware rule-engine is less flexible than a table look-up approach, unless a software layer can be added to customize the rule engine for a choice of several different rule sets.

Since many lattice points reside on each chip, and since off-chip communications are slower than those that remain on-chip, it seems desirable to locate on each chip the look-up tables or hardware rule-engines which calculate the collision outcomes. This avoids the time delays which would occur if one had to go off-chip to calculate collision outcomes. If there are many

lattice points on a chip, one may want to have many "computational nodes" on each chip. (Here a "computational node" is defined to be a look-up table or a rule-engine for calculating collision outcomes.) This would avoid the time delays inherent in updating all of the lattice points on a given chip sequentially.

Thus one must choose how to trade off the number of lattice points which can be stored on a chip with the number of "computational nodes" that will fit on a chip. The results of this trade-off will probably vary with the specific type of rule set chose, since the size and complexity of the "computational node" and the number of bits required for a lattice point will in general vary. In the example shown in the following table, it was decided to allocate half of the chip space to lattice points and half to "computational nodes."

With the above discussion as background, the workshop arrived at the following the target performance characteristics of a hypothetical lattice-gas computer:

Table 2: Target Performance Parameters

Problem definition:
Three-dimensional incompressible hydrodynamics
Flexible boundary conditions
Some flexibility in the rule set
If possible, high input-output rate
Hardware aspects:
512 lattice points per "computational node"
64 "computational nodes" per chip
32,000 lattice points per chip
About a million chips total
3×10^{10} lattice points total ($> 10^{11}$ within 5 years)
10 nsec update rate (on-chip)
About 64×10^{8} site updates per chip per second
About 6×10^{15} site updates/sec total
($> 6 \times 10^{16}$ site updates/sec within 5 years)

5 CONCLUSIONS

The workshop in La Jolla produced a considerable amount of enthusiasm about the potential of a dedicated special-purpose lattice-gas computer. Preliminary estimates based on the above performance numbers suggest that such a machine could surpass the present performance of a general-purpose supercomputer such as the Cray II (3×10^7 site updates/sec) by a factor of about 10^8 and possibly considerably more. Of course the target machine could be expensive; first-of-a-kind supercomputers can cost from tens to a hundred million dollars. The cost of this machine is proportional to the number of chips, so a reduction in chip count by a factor of 10 would result in a factor of 10 reduction in cost.

In view of the combination of large cost and high scientific potential for such a machine, it will be imperative to proceed along two parallel paths: 1) refinement of the theoretical understanding of cellular automata rules and lattices in three spatial dimensions, and 2) building of intermediate-scale hardware implementations of dedicated cellular automata computational engines, so as to gain expertise in the practical areas of architecture tradeoffs and implementations. A very good example of such an intermediate engine is the CAM-8 machine recently proposed by Margolus and Toffoli, which would deliver 2×10^{10} site updates per second with 16 bits per site. Progress along both of these paths will be necessary in order to learn how to best exploit the potential of a dedicated lattice-gas supercomputer.

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